

Flexing of a Carbon Nanotube

NRL molecular dynamics simulation of the 90 ps oscillation of a 30-nm-long multiwall carbon nanotube composed of over 12,000 atoms. The nanotube consists of an inner semiconducting chiral tubule with radii of 0.69 nm and 1.03 nm, respectively. The initial conditions for the simulation were obtained by bending and relaxing the tube past the point it buckled and then releasing one of its ends.